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PGSCM: A family of P -stable Boundary Value Methods for second-order initial value problems

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ABSTRACT

In this paper, we introduce a family of Linear Multistep Methods used as Boundary Value Methods for the numerical solution of initial value problems for second order ordinary differential equations of special type. We rigorously prove that these schemes are P -stable, in a generalized sense, of arbitrarily high order. This overcomes the barrier that Lambert and Watson established in Lambert and Watson (1976) [1] on Linear Multistep Methods used in the classic way; that is as Initial Value Methods. We call the new methods PGSCMs, an acronym for P_v -stable Generalized Störmer–Cowell Methods. Numerical illustrations which confirm the theoretical results of the paper are finally given.

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1. Introduction

The numerical solution of initial value problems for second order ordinary differential equations of special type given by

$$y''(x) = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad x \in [x_0, X], \quad (1)$$

having periodic and oscillatory solution $y(x) \in \mathbb{R}^r$, has attracted much interest in recent decades. It is well-known that these problems can be easily reformulated as systems of first order ODEs of size $2r$ so that one of the several schemes currently available in the literature for the latter type of problems can be applied for their solution. It is evident, however, that the use of numerical schemes designed for solving (1) in its original formulation is more competitive from the point of view of the computational complexity.

In this context, the application of Linear Multistep Methods (LMMs) is one of the classical approaches. If the interval of integration is discretized with a uniform partition with stepsize $h = (X - x_0)/N$, then a k -step LMM with coefficients α_j 's and β_j 's replaces the equation in (1) with the following difference equation

$$\sum_{j=0}^k \alpha_j y_{n+j} = h^2 \sum_{j=0}^k \beta_j f_{n+j}, \quad (2)$$

where $y_n \approx y(x_n)$, $f_n = f(x_n, y_n)$, with $x_n = x_0 + nh$, for all $n = 0, 1, \dots, N$.

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In this paper we will focus our attention to problems exhibiting *periodic stiffness* [1,2]. This happens when their solutions are a combination of components with dominant short frequencies and components with large frequencies and negligible amplitudes. In particular, we will consider the case where one is interested in reproducing only the low-frequency components of the solution and the high-frequency components represent a perturbation. To this end, the use of schemes satisfying “good” stability properties is mandatory. In [1] Lambert and Watson propose a linear stability analysis of (2) based on the following test equation

$$y'' = -\lambda^2 y, \quad \lambda \in \mathbb{R}, \quad (3)$$

whose general exact solution, given by $y(x) = A \cos(\lambda x) + B \sin(\lambda x)$, is periodic with period $2\pi/\lambda$ (actually with the only exception of the cases $\lambda = 0$ or $A = B = 0$). The aim of this analysis is to find, following the classical idea of Dahlquist, the conditions for which the corresponding numerical solution has (essentially) the same qualitative behavior as the continuous one.

This led to the definition of interval of periodicity and of P -stability of a method which ensures that the numerical solution has the desired behavior independently of the used stepsize. In the same paper, however, the authors established that the order of a P -stable LMM, used as Initial Value Method (IVM), cannot exceed two which is exactly the analogous of the famous second Dahlquist barrier.

In order to overcome this undeniable negative result, in the frame of linear multistep methods, a number of approaches has been adopted across the years. Among them, we mention the hybrid methods proposed in [3–5], the super-implicit and Obrechhoff methods discussed in [6–8] and the class of symmetric two-step Obrechhoff methods recently studied by Van Daele and Vanden Berghen in [9]. In particular, the latter ones are P -stable schemes of order $p = 2m$, with $m \in \mathbb{N}$, which make use of the derivatives of the unknown solution up to order $2m$. In addition, in the last years, particular attention has been devoted to exponential-fitting methods (see, for example, [10–13]) which is a surely interesting field of research.

In this article, we shall investigate if the use of LMMs as Boundary Value Methods (BVMs) is successful in overcoming the barrier of Lambert and Watson. The main idea on which such schemes rely is that of completing the discrete problem generated by a LMM with a set of boundary conditions instead of just initial ones as classically done. This approach was introduced in the nineties for the definition of schemes for solving first order ODEs and the principal reference is [14]. Their linear stability properties have been studied in detail in several papers where it is proved rigorously that they are able to overcome the second Dahlquist barrier [15–20].

The article is organized as follows. In Section 2 we recall the definitions of interval of periodicity and of P -stability for IVMs and we give their generalization to the case where the LMMs are used as BVMs. In Section 3 we introduce a family of BVMs, that we call PGSCMs, and we prove some properties of their coefficients. The linear stability analysis of the new methods is carried out in Section 4 where it is proved that they are P -stable formulae, in the sense corresponding to BVMs, of arbitrarily high order. Finally, in Section 5 we propose additional formulae to be coupled with the main LMM in order to recover the boundary values required by the discrete problem. The results of some numerical experiments conducted with the new schemes are also reported which confirm the theory of the previous sections.

2. P -stability for initial and boundary value methods

When the method (2) is applied for solving (3) the discrete problem reduces to the following linear difference equation

$$\sum_{j=0}^k \alpha_j y_{n+j} + q^2 \sum_{j=0}^k \beta_j y_{n+j} = 0, \quad q = h\lambda.$$

The corresponding stability polynomial is

$$\pi(z, q^2) = \rho(z) + q^2 \sigma(z),$$

where, as usual,

$$\rho(z) = \sum_{j=0}^k \alpha_j z^j, \quad \sigma(z) = \sum_{j=0}^k \beta_j z^j$$

are the characteristic polynomials of the method. As is well-known, such a method is consistent if

$$\rho(1) = \rho'(1) = 0, \quad \rho''(1) = 2\sigma(1). \quad (4)$$

Before proceeding, we recall the following definition of type of a polynomial [21].

Definition 1. A polynomial is said to be of type (m_1, m_2, m_3) if it has m_1, m_2 and m_3 roots inside, on the boundary, and outside the unit circle in the complex plane, respectively.

Let, from now on, $z_1(q^2), z_2(q^2), \dots, z_k(q^2)$ be the roots of $\pi(z, q^2)$ ordered with increasing modulus. When the LMM is used as IVM, namely when the discrete problem (2) is completed by fixing the values of $y_0, y_1, \dots, y_{k-1}, z_{k-1}(q^2) = z_k(q^2)$ are the principal roots of the method; that is, $z_{k-1}(0) = z_k(0) = 1$.

It is well-known that, if $|z_{k-2}(q^2)| < |z_{k-1}(q^2)|$ then the solution provided by an IVM is essentially given by a linear combination of $z_{k-1}^n(q^2)$ and $z_k^n(q^2)$. This led Lambert and Watson to give the definitions of interval of periodicity and of P -stability which we report here rewritten in an equivalent form by using the notation given in Definition 1.

Definition 2. A k -step IVM has interval of periodicity $I = (0, q_0^2)$, if $q^2 \in I$ implies that its stability polynomial $\pi(z, q^2)$ is of type $(k - m, m, 0)$ where $m = m(q^2)$ with $2 \leq m(q^2) \leq k$.

Definition 3. An IVM is P -stable if $I = (0, \infty)$ being I its interval of periodicity.

If the LMM has a nonempty interval of periodicity, then, by using h such that $q^2 \in I$, the numerical solution has the desired qualitative behavior on the test equation. This is the case, for example, of the famous Numerov method,

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{12} (f_{n+2} + 10f_{n+1} + f_n),$$

which has interval of periodicity $(0, 6)$. A similar restriction on the stepsize does not occur if the method used is P -stable and this is surely mandatory if the problem to be solved is stiff. For example, the following methods introduced in [1]

$$y_{n+2} - 2y_{n+1} + y_n = \frac{h^2}{2 - 2\cos\phi} (f_{n+2} - 2\cos\phi f_{n+1} + f_n) \quad (5)$$

have order two and are P -stable for all $\phi \in (0, 2\pi)$. However, as stated in the same paper, the order of accuracy of a P -stable LMM used as IVM cannot exceed two.

In this paper we shall investigate if the use of the BVM approach allows to overcome such barrier. In this case a set of boundary conditions is associated to the difference Eq. (2). More precisely, when applied for solving (1), the discrete problem generated by a k -step BVM used with (k_1, k_2) -boundary conditions, $k_1 + k_2 = k$, is given by (2) coupled with

$$y_0, y_1, \dots, y_{k_1-1}, \quad y_{N-k_2+1}, \dots, y_N \quad \text{fixed.} \quad (6)$$

We shall talk in Section 5 about a possible strategy that can be used for getting an approximation of the boundary values. The important advantage that arises from this approach is that the principal roots of the method are no longer restricted to be the ones of largest modulus. This is a consequence of the following result.

Theorem 1. Suppose that a linear difference equation of order k with constant coefficients has characteristic roots z_i satisfying

$$|z_1| \leq \dots \leq |z_{k_1-2}| < |z_{k_1-1}| = |z_{k_1}| < |z_{k_1+1}| \leq \dots \leq |z_k|, \quad 1 < |z_{k_1+1}|,$$

with $z_{k_1-1} \neq z_{k_1}$. Then, the solution of an associated boundary value problem with k_1 initial values and $k_2 = k - k_1$ final ones as in (6) behaves as

$$y_n = |z_{k_1}|^n \left[\hat{\gamma}_1 \left(\frac{z_{k_1-1}}{|z_{k_1-1}|} \right)^n + \hat{\gamma}_2 \left(\frac{z_{k_1}}{|z_{k_1}|} \right)^n + O \left(\left| \frac{z_{k_1-2}}{z_{k_1}} \right|^n \right) + O \left(\left| \frac{z_{k_1}}{z_{k_1+1}} \right|^{N-n} \right) + O(|z_{k_1+1}|^{-N}) \right] + O(|z_{k_1+1}|^{-(N-n)}),$$

when n and $N - n$ are sufficiently large. In the previous asymptotic estimate, the coefficients $\hat{\gamma}_1$ and $\hat{\gamma}_2$ depend only on the initial values $y_0, y_1, \dots, y_{k_1-1}$.

Proof. The statement can be proved by using arguments similar to the ones considered in the proof of Theorem 2.6.1 in [14]. \square

Clearly, from the previous theorem one gets that, for a fixed $q^2 > 0$, the numerical solution provided by a k -step BVM with (k_1, k_2) -boundary conditions is (essentially) periodic if $\pi(z, q^2)$ is of type $(k_1 - 2, 2, k_2)$. In this regard, in [1] it was proved that this may happen only if the method is symmetric, i.e.

$$\alpha_j = \alpha_{k-j}, \quad \beta_j = \beta_{k-j}, \quad j = 0, 1, \dots, k.$$

In the same paper, it was also proved that a symmetric irreducible LMM has stepnumber and order even. In the sequel, we shall therefore assume $k = 2\nu$ with $\nu \geq 1$. We can now give the following definitions which extend the ones given for an IVM.

Definition 4. A (2ν) -step BVM with $(\nu + 1, \nu - 1)$ -boundary conditions is said to have interval of ν -periodicity $I_\nu = (0, q_0^2)$, if $\pi(z, q^2)$ is of type $(\nu - 1, 2, \nu - 1)$ for all $q^2 \in I_\nu$.

Definition 5. A (2ν) -step BVM with $(\nu + 1, \nu - 1)$ -boundary conditions is said P_ν -stable if $I_\nu = (0, \infty)$.

The main target of this article is to determine a family of P_v -stable BVMs of order greater than two, i.e. methods that overcome the barrier established by Lambert and Watson in [1]. The tool that we are going to use for the linear stability analysis is the boundary locus of the method defined by

$$\Gamma = \left\{ q^2 \in \mathbb{C} : q^2 \equiv \psi(\theta) = -\frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}, \theta \in [0, 2\pi) \right\}. \quad (7)$$

It is not difficult to verify that

- the elements of Γ are the values of q^2 such that $\pi(z, q^2)$ has at least one root on the unit circle;
- if the method is symmetric then $\Gamma \subset \mathbb{R}$, $\psi(\theta) = \psi(2\pi - \theta) = \psi(-\theta)$;
- $I_v \subseteq \Gamma$ so that a $(2v)$ -step BVM can be P_v -stable only if Γ is unbounded, i.e. if there exists $\theta \in (0, 2\pi)$ such that $\sigma(e^{i\theta}) = 0$.

3. PGSCMs for second order ODEs

In this section, we shall derive a family of BVMs obtained as a generalization of the popular Störmer–Cowell methods, [22]. They verify the necessary conditions to be P_v -stable, namely their boundary locus is unbounded and they are symmetric. The first property is verified by construction while the second one will be proved after their derivation. We name these schemes PGSCMs, an acronym for *P_v -stable Generalized Störmer–Cowell Methods*.

When applied for solving (1), the difference equation generated by the $(2v)$ -step PGSCM reads

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \sum_{j=-v}^v \beta_{j+v}^{(2v)} f_{n+j}, \quad n = v, v+1, \dots, N-v, \quad (8)$$

with $v \in \mathbb{N}$. Observe that we have introduced an upper index on the coefficients β_j 's to denote the stepnumber of the corresponding method. As for the Störmer–Cowell methods, these formulae have the first characteristic polynomial

$$\rho_{2v}(z) = \sum_{j=0}^{2v} \alpha_j^{(2v)} z^j = z^{v-1} (z-1)^2 \quad (9)$$

fixed a priori which verifies the first two consistency conditions $\rho_{2v}(1) = \rho'_{2v}(1) = 0$, see (4). The second characteristic polynomial

$$\sigma_{2v}(z) = \sum_{j=0}^{2v} \beta_j^{(2v)} z^j \quad (10)$$

is determined by imposing the formula to have order $p = 2v$ and

$$\sigma_{2v}(-1) = 0, \quad (11)$$

so that the associated boundary locus (7) is unbounded. The method has order $p = 2v$ if the following order conditions, obtained by considering the Taylor series expansion of the exact solution at $x = x_v$, are verified

$$\sum_{j=-v}^v \beta_{j+v}^{(2v)} j^{s-2} = \frac{(-1)^s + 1}{s(s-1)}, \quad s = 2, 3, \dots, 2v+1. \quad (12)$$

It is important to observe that the so-obtained 2-step method coincides with the one in (5) corresponding to $\phi = \pi$ so that the family of PGSCMs represents a generalization of it. In addition, the 4-step method has been already derived in [23] even though its stability properties were not proved in such paper.

With the aim of writing (11)–(12) in matrix form, we introduce the following notation. For each $\ell \geq 1$ and $x \in \mathbb{R}$, let

$$\xi_\ell(x) = (x^0, x^1, \dots, x^{\ell-1})^T. \quad (13)$$

In addition, let

$$V = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -v & -v+1 & \cdots & v \\ \vdots & \vdots & \ddots & \vdots \\ (-v)^{2v} & (-v+1)^{2v} & \cdots & v^{2v} \end{pmatrix}, \quad (14)$$

$$\mathbf{v}_{2v} = \left(\frac{2}{2 \cdot 1}, 0, \frac{2}{4 \cdot 3}, 0, \dots, \frac{2}{2v \cdot (2v-1)}, 0 \right)^T, \quad (15)$$

$$\tilde{I} = \begin{pmatrix} I_{2v} & \mathbf{0}_{2v} \\ \mathbf{0}_{2v}^T & 0 \end{pmatrix}, \quad E = \begin{pmatrix} O_{2v} & \mathbf{0}_{2v} \\ \xi_{2v}^T(-1) & 1 \end{pmatrix}, \quad (16)$$

where $I_{2\nu}$, $O_{2\nu}$ and $\mathbf{0}_{2\nu}$ are the identity matrix, the zero matrix and the zero vector of size 2ν , respectively. Then, one verifies that (11)–(12) can be reformulated in matrix form as

$$(\tilde{V} + E)\boldsymbol{\beta}^{(2\nu)} = \begin{pmatrix} \mathbf{v}_{2\nu} \\ 0 \end{pmatrix} \quad (17)$$

where $\boldsymbol{\beta}^{(2\nu)} = (\beta_0^{(2\nu)}, \beta_1^{(2\nu)}, \dots, \beta_{2\nu}^{(2\nu)})^T$. The methods obtained as just described satisfy the following proposition.

Proposition 1. For each $\nu \geq 1$, the coefficient vector $\boldsymbol{\beta}^{(2\nu)}$ of the (2ν) -step PGSCM (8) satisfying (11)–(12) is unique. Moreover, the method is symmetric, namely, by denoting with J the anti-identity matrix of size $2\nu + 1$, its coefficient vectors satisfy

$$\boldsymbol{\alpha}^{(2\nu)} = J\boldsymbol{\alpha}^{(2\nu)}, \quad \boldsymbol{\beta}^{(2\nu)} = J\boldsymbol{\beta}^{(2\nu)}, \quad (18)$$

where $\boldsymbol{\alpha}^{(2\nu)} = (\alpha_0^{(2\nu)}, \alpha_1^{(2\nu)}, \dots, \alpha_{2\nu}^{(2\nu)})^T$ has all zero entries with the exception of $\alpha_{\nu-1}^{(2\nu)} = \alpha_{\nu+1}^{(2\nu)} = 1$ and $\alpha_\nu^{(2\nu)} = -2$.

Proof. By applying the Laplace expansion along the last row and using the fact that the determinant of a Vandermonde matrix with increasing abscissae is positive, it is not difficult to verify that the coefficient matrix $\tilde{V} + E$ of system (17) has a positive determinant so that $\boldsymbol{\beta}^{(2\nu)}$ is uniquely determined.

Concerning the symmetry of the method, the first relation in (18) is trivially verified by construction while, in view of the uniqueness of the method, the second relation holds true if $\boldsymbol{\beta}^{(2\nu)}$ and $J\boldsymbol{\beta}^{(2\nu)}$ are both solutions of (17). We observe that, see (13)–(16), $\tilde{V}J = \text{diag}(\xi_{2\nu+1}(-1))\tilde{V}$ and $EJ = \text{diag}(\xi_{2\nu+1}(-1))E$. This implies

$$\begin{aligned} (\tilde{V} + E)J\boldsymbol{\beta}^{(2\nu)} &= \text{diag}(\xi_{2\nu+1}(-1))(\tilde{V} + E)\boldsymbol{\beta}^{(2\nu)} \\ &= \text{diag}(\xi_{2\nu+1}(-1)) \begin{pmatrix} \mathbf{v}_{2\nu} \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{2\nu} \\ 0 \end{pmatrix}, \end{aligned}$$

where, see (15), the last equality is due to the fact that the entries with even index in $\mathbf{v}_{2\nu}$ are all zero. The vector $J\boldsymbol{\beta}^{(2\nu)}$ is therefore a solution of (17) and this completes the proof. \square

In Table 1 the normalized coefficients $\hat{\beta}_j^{(2\nu)} = \eta_{2\nu}\beta_j^{(2\nu)}$, $j = 0, 1, \dots, \nu$ have been reported for $\nu = 1, 2, 3, 4$.

3.1. Properties of the second characteristic polynomial

The first result we are going to prove is that the second characteristic polynomials of PGSCMs are related by a recurrence relation and to this aim we need the following lemma.

Lemma 1. For each integer m , let $P = (p_{ij})_{i,j=1,\dots,m}$ be the lower triangular Pascal matrix whose nonzero entries are

$$p_{ij} = \binom{i-1}{j-1}, \quad 1 \leq j \leq i \leq m,$$

and let

$$H = \begin{pmatrix} \mathbf{0}^T & 0 \\ I_{m-1} & \mathbf{0} \end{pmatrix}. \quad (19)$$

Then, for each $\ell = 1, \dots, m-1$,

$$P^T H^\ell = (I_m + H)^\ell P^T + R_\ell, \quad (20)$$

where R_ℓ has the first $m - \ell$ columns with all zero entries.

Proof. We proceed by induction on ℓ . If $\ell = 1$ we verify the statement by direct inspection. In fact,

$$(P^T H)_{ij} = \binom{j}{i-1} = \binom{j-1}{i-1} + \binom{j-1}{i-2} = (P^T)_{ij} + (HP^T)_{ij}, \quad j = 1, 2, \dots, m-1, \quad i = j, j+1, \dots, m.$$

This implies that, when $\ell = 1$, (20) is verified with R_1 a suitable matrix having the first $m - 1$ columns with all zero entries.

Next, by induction, if it holds true for ℓ it holds true also for $\ell + 1$. In fact, from the induction hypothesis and by taking into account that $P^T H = (I_m + H)P^T + R_1$, as just proved, we obtain

$$\begin{aligned} P^T H^{\ell+1} &= (I_m + H)^\ell P^T H + R_\ell H \\ &= (I_m + H)^{\ell+1} P^T + (I_m + H)^\ell R_1 + R_\ell H \\ &\equiv (I_m + H)^{\ell+1} P^T + R_{\ell+1}, \end{aligned}$$

where $R_{\ell+1}$ has the first $m - \ell - 1$ columns with all zero entries. \square

Table 1
Normalized coefficients of PGSCMs.

ν	$\eta_{2\nu}$	$\hat{\beta}_0^{(2\nu)}$	$\hat{\beta}_1^{(2\nu)}$	$\hat{\beta}_2^{(2\nu)}$	$\hat{\beta}_3^{(2\nu)}$	$\hat{\beta}_4^{(2\nu)}$
1	4	1	2			
2	24	−1	6	14		
3	960	9	−58	231	596	
4	60 480	−134	1103	−4190	14 017	38 888

We can now state the following theorem.

Theorem 2. The second characteristic polynomials of PGSCMs verify the recurrence relation

$$\sigma_2(z) = \gamma_1(z+1)^2 \equiv \frac{1}{4}(z+1)^2, \quad (21)$$

$$\sigma_{2\nu}(z) = z \sigma_{2\nu-2}(z) + \gamma_\nu(z-1)^{2\nu-2}(z+1)^2, \quad \nu = 2, 3, \dots, \quad (22)$$

for suitable coefficients γ_ν , $\nu \geq 2$.

Proof. Concerning (21) nothing has to be proved (see Table 1). With reference to (22), the relation holds true if $\beta^{(2\nu)}$ can be written in the form

$$\beta^{(2\nu)} = \begin{pmatrix} 0 \\ \beta^{(2\nu-2)} \\ 0 \end{pmatrix} + \gamma_\nu \mathbf{c}^{(\nu)} \quad (23)$$

where γ_ν is a suitable coefficient and $\mathbf{c}^{(\nu)} = (c_0^{(\nu)}, c_1^{(\nu)}, \dots, c_{2\nu}^{(\nu)})^T$ satisfies, see (13),

$$(z-1)^{2\nu-2}(z+1)^2 = \sum_{i=0}^{2\nu} c_i^{(\nu)} z^i = \xi_{2\nu+1}^T(z) \mathbf{c}^{(\nu)}. \quad (24)$$

From (17) one gets that (23) is equivalent to

$$(\tilde{I}V + E) \begin{pmatrix} 0 \\ \beta^{(2\nu-2)} \\ 0 \end{pmatrix} - \begin{pmatrix} \mathbf{v}_{2\nu} \\ 0 \end{pmatrix} = -\gamma_\nu (\tilde{I}V + E) \mathbf{c}^{(\nu)}. \quad (25)$$

Now, it results

$$(\tilde{I}V + E) \begin{pmatrix} 0 \\ \beta^{(2\nu-2)} \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{v}_{2\nu-2} \\ \chi \\ 0 \\ 0 \end{pmatrix},$$

for a suitable $\chi \in \mathbb{R}$. In fact, the first $2\nu-2$ of the previous equalities and the last one are the conditions (17), with $\nu-1$ in place of ν , which uniquely determine $\beta^{(2\nu-2)}$. The second last equality, instead, is due to the symmetry of the $(2\nu-2)$ -step method. In addition, see (15),

$$\mathbf{v}_{2\nu} = \begin{pmatrix} \frac{\mathbf{v}_{2\nu-2}}{2} \\ 2\nu \cdot (2\nu-1) \\ 0 \end{pmatrix}.$$

This implies that the vector on the left hand-side in (25) belongs to $\text{span}\{\mathbf{e}_{2\nu-1}\}$ where, from now on, \mathbf{e}_ℓ will denote the ℓ -th unit vector of size $2\nu+1$. It follows that Eq. (25) holds true if $(\tilde{I}V + E)\mathbf{c}^{(\nu)} \in \text{span}\{\mathbf{e}_{2\nu-1}\}$. From (16) and (24), one gets $E\mathbf{c}^{(\nu)} = \mathbf{0}_{2\nu+1}$ so that it remains to verify that $\tilde{I}V\mathbf{c}^{(\nu)} \in \text{span}\{\mathbf{e}_{2\nu-1}\}$ or, equivalently, that $V\mathbf{c}^{(\nu)} \in \text{span}\{\mathbf{e}_{2\nu-1}, \mathbf{e}_{2\nu+1}\}$.

It is known that the Vandermonde matrix V can be decomposed as [24]

$$V = P^{-\nu} S D_f P^T,$$

where P is the Pascal matrix of size $2\nu+1$ given in Lemma 1, S is the unit lower triangular matrix of order $2\nu+1$ whose nonzero entries are the Stirling numbers of the second kind and $D_f = \text{diag}(0!, 1!, \dots, (2\nu)!)$. Therefore, if we let $\mathbf{w}_\nu = P^T \mathbf{c}^{(\nu)}$, then we need to verify that

$$P^{-\nu} S D_f \mathbf{w}_\nu \in \text{span}\{\mathbf{e}_{2\nu-1}, \mathbf{e}_{2\nu+1}\}.$$

It is known that the nonzero entries of P^{-T} are given by [24]

$$(P^{-T})_{ij} = \binom{j-1}{i-1} (-1)^{i-j}, \quad 1 \leq i \leq j \leq 2\nu + 1$$

from which, see (13) and (19), one gets

$$z^\ell (z-1)^{2\nu-2} = (\xi_{2\nu+1}^T(z) H^\ell) P^{-T} \mathbf{e}_{2\nu-1}, \quad \ell = 0, 1, 2.$$

The coefficient vector $\mathbf{c}^{(\nu)}$ in (24) can be therefore written as

$$\mathbf{c}^{(\nu)} = (I_{2\nu+1} + 2H + H^2) P^{-T} \mathbf{e}_{2\nu-1}$$

so that, from (20) and considering that the last two entries of $P^{-T} \mathbf{e}_{2\nu-1}$ are zero, we get

$$\begin{aligned} \mathbf{w}_\nu &= P^T \mathbf{c}^{(\nu)} = (I + 2(I+H) + (I+H)^2 + 2R_1 P^{-T} + R_2 P^{-T}) \mathbf{e}_{2\nu-1} \\ &= 4\mathbf{e}_{2\nu-1} + 4\mathbf{e}_{2\nu} + \mathbf{e}_{2\nu+1}. \end{aligned}$$

By virtue of the fact that $P^{-\nu} S D_f$ is lower triangular, we then obtain

$$P^{-\nu} S D_f \mathbf{w}_\nu \in \text{span}\{\mathbf{e}_{2\nu-1}, \mathbf{e}_{2\nu}, \mathbf{e}_{2\nu+1}\}.$$

The result is therefore proved if $\mathbf{e}_{2\nu}^T P^{-\nu} S D_f \mathbf{w}_\nu = 0$, i.e. if

$$\begin{aligned} \mathbf{e}_{2\nu}^T P^{-\nu} S D_f \mathbf{w}_\nu &= 4\mathbf{e}_{2\nu}^T P^{-\nu} S D_f (\mathbf{e}_{2\nu-1} + \mathbf{e}_{2\nu}) \\ &= 4(2\nu-2)! \mathbf{e}_{2\nu}^T P^{-\nu} S (\mathbf{e}_{2\nu-1} + (2\nu-1)\mathbf{e}_{2\nu}) \\ &= 4(2\nu-2)! (\mathbf{e}_{2\nu}^T P^{-\nu} S \mathbf{e}_{2\nu-1} + 2\nu-1) = 0, \end{aligned}$$

but the latter equality holds true since $P^{-\nu}$ and S are both unit lower triangular and [24,25]

$$(P^{-\nu})_{2\nu, 2\nu-1} = -\nu \binom{2\nu-1}{2\nu-2}, \quad (S)_{2\nu, 2\nu-1} = \binom{2\nu-1}{2}$$

so that

$$\mathbf{e}_{2\nu}^T P^{-\nu} S \mathbf{e}_{2\nu-1} = (P^{-\nu})_{2\nu, 2\nu-1} + (S)_{2\nu, 2\nu-1} = 1 - 2\nu. \quad \square$$

Remark 1. For each $\nu \geq 1$, the coefficient γ_ν in (21)–(22) is the leading coefficient of $\sigma_{2\nu}(z)$. This clearly implies $\gamma_\nu = \beta_{2\nu}^{(2\nu)}$.

We are now going to establish some properties of the coefficient $\beta_{2\nu}^{(2\nu)}$. If we apply the Cramer method to (17), we get

$$\beta_{2\nu}^{(2\nu)} = \frac{\det(W)}{\det(\tilde{I}V + E)}$$

where W is obtained from $\tilde{I}V + E$ by replacing its last column with the vector of constant terms. It can be verified by direct inspection that $\tilde{I}V + E$ can be factorized as

$$\tilde{I}V + E \equiv \begin{pmatrix} \hat{V} & \xi_{2\nu}(\nu) \\ \xi_{2\nu}^T(-1) & 1 \end{pmatrix} = \begin{pmatrix} I_{2\nu} & \mathbf{0}_{2\nu} \\ \xi_{2\nu}^T(-1) \hat{V}^{-1} & 1 \end{pmatrix} \begin{pmatrix} \hat{V} & \xi_{2\nu}(\nu) \\ \mathbf{0}_{2\nu}^T & 1 - \xi_{2\nu}^T(-1) \hat{V}^{-1} \xi_{2\nu}(\nu) \end{pmatrix},$$

where, see (14), $\hat{V} \in \mathbb{R}^{(2\nu) \times (2\nu)}$ is obtained from V by removing its last row and column. It follows that $\det(\tilde{I}V + E) = \det(\hat{V})(1 - \xi_{2\nu}^T(-1) \hat{V}^{-1} \xi_{2\nu}(\nu))$. With a similar factorization for W one gets $\det(W) = -\det(\hat{V})(\xi_{2\nu}^T(-1) \hat{V}^{-1} \mathbf{v}_{2\nu})$. Therefore,

$$\beta_{2\nu}^{(2\nu)} = \frac{\xi_{2\nu}^T(-1) \hat{V}^{-1} \mathbf{v}_{2\nu}}{\xi_{2\nu}^T(-1) \hat{V}^{-1} \xi_{2\nu}(\nu) - 1}. \quad (26)$$

We observe that the entries of $\hat{V}^{-T} \xi_{2\nu}(-1)$ can be read as the coefficients with respect to the monomial basis of the polynomial $p_\nu(t) = \xi_{2\nu}^T(-1) \hat{V}^{-1} \xi_{2\nu}(t) \in \Pi_{2\nu-1}$ that interpolates the following data set

$$p_\nu(j) = (-1)^{j+\nu}, \quad j = -\nu, 1-\nu, \dots, \nu-1. \quad (27)$$

This clearly implies that the denominator in (26) is equal to $p_\nu(\nu) - 1$. Concerning the numerator, one may verify that, see (13)–(15)

$$\xi_{2\nu}^T(-1) \hat{V}^{-1} \mathbf{v}_{2\nu} = \xi_{2\nu}^T(-1) \hat{V}^{-1} \int_0^1 \int_0^x (\xi_{2\nu}(t) + \xi_{2\nu}(-t)) dt dx = \int_0^1 \int_0^x (p_\nu(t) + p_\nu(-t)) dt dx.$$

From all these considerations, we obtain that (26) can be rewritten as

$$\beta_{2\nu}^{(2\nu)} = \frac{\int_0^1 \int_{-x}^x p_\nu(t) dt dx}{p_\nu(\nu) - 1}. \quad (28)$$

In order to prove some properties of $\beta_{2\nu}^{(2\nu)}$ we need the results concerning the polynomial $p_\nu(t)$ stated in the following lemma.

Lemma 2. For each $\nu \geq 1$, the polynomial $p_\nu(t) \in \Pi_{2\nu-1}$ that interpolates the data set (27) satisfies the following properties:

P1. $p_\nu(\nu) - 1 = -4^\nu$;

P2. the leading coefficient of $p_\nu(t)$, say ω_ν , is negative;

P3. $p_\nu(t)$ is symmetric with respect to $t = -\frac{1}{2}$, i.e. $p_\nu(-1/2 + t) + p_\nu(-1/2 - t) = 0$ for all $t \in \mathbb{R}$;

P4. $(-1)^\nu \int_{-x}^x p_\nu(t) dt > 0$, for all $x \in (0, 1)$;

P5. $(-1)^\nu \int_{-x}^x (p_\nu(t) + p_{\nu+1}(t)) dt \geq 0$, for all $x \in [0, 1]$.

Proof. Concerning property **P1**, by using the Lagrange basis for the interpolating polynomial, we get

$$p_\nu(t) = \sum_{j=-\nu}^{\nu-1} (-1)^{j+\nu} \ell_j(t), \quad \ell_j(t) = \prod_{i=-\nu, i \neq j}^{\nu-1} \frac{t-i}{j-i}.$$

Now, one may verify that

$$\ell_j(\nu) = \prod_{i=-\nu, i \neq j}^{\nu-1} \frac{\nu-i}{j-i} = \frac{(2\nu)!}{(\nu-j)(\nu+j)!(\nu-j-1)!} (-1)^{\nu-j-1} = (-1)^{\nu-j-1} \binom{2\nu}{\nu+j}$$

and, consequently,

$$p_\nu(\nu) - 1 = - \left(\sum_{j=-\nu}^{\nu-1} \binom{2\nu}{\nu+j} \right) - 1 = - \sum_{j=0}^{2\nu} \binom{2\nu}{j} = -4^\nu.$$

The property **P2** is a consequence of the fact that $p_\nu \in \Pi_{2\nu-1}$, $p_\nu(-\nu) = 1$ and the zeros of $p_\nu(t)$ are all real and belong to $[-\nu, \nu-1]$ since in such interval $p_\nu(t)$ changes sign $2\nu-1$ times. This implies $\lim_{t \rightarrow -\infty} p_\nu(t) = +\infty$, i.e. $\omega_\nu < 0$.

In order to prove **P3**, it suffices to observe that $p_\nu(-1/2 + t_j) + p_\nu(-1/2 - t_j) = 0$, for $t_j = -\nu - \frac{1}{2} + j$ with $j = 1, 2, \dots, 2\nu$ which implies that $p_\nu(-1/2 + t) + p_\nu(-1/2 - t)$ is the zero polynomial.

Concerning **P4**, notice that $p_\nu(t) \in \Pi_{2\nu-1}$, $\omega_\nu < 0$ and, see (27), $p_\nu(j) - p_\nu(-j) = 0$, for each $j = 1 - \nu, \dots, \nu - 1$. Consequently, $p_\nu(t) - p_\nu(-t) = 2\omega_\nu \prod_{j=1-\nu}^{\nu-1} (t-j)$ and therefore

$$(-1)^\nu (p_\nu(t) - p_\nu(-t)) > 0, \quad \text{for all } t \in (0, 1). \quad (29)$$

This implies that if $x \in (0, 1)$ then

$$(-1)^\nu \int_{-x}^x p_\nu(t) dt > (-1)^\nu \left(\int_0^x p_\nu(-t) dt + \int_{-x}^0 p_\nu(t) dt \right) = (-1)^\nu 2 \int_{-x}^0 p_\nu(t) dt \geq 0,$$

where the last inequality is due to property **P3** and to the facts that $p_\nu(0) = (-1)^\nu$ and, when $t \in [-1, 0]$, $p_\nu(t) = 0$ only for $t = -\frac{1}{2}$.

Finally, in order to obtain property **P5** we proceed by applying arguments similar to the ones used for proving the inequality in (29). In fact, by letting $q_\nu(t) = p_\nu(t) + p_{\nu+1}(t) \in \Pi_{2\nu+1}$, from (27) and property **P3** we get $q_\nu(j) = 0$, for each $j = -\nu, \dots, \nu-1, -\frac{1}{2}$, i.e.

$$q_\nu(t) = \omega_{\nu+1} \left(t + \frac{1}{2} \right) \prod_{j=-\nu}^{\nu-1} (t-j) = \omega_{\nu+1} t \left(t + \frac{1}{2} \right) (t+\nu) \prod_{j=1}^{\nu-1} (t^2 - j^2),$$

where we recall that $\omega_{\nu+1} < 0$ represents the leading coefficient of $p_{\nu+1}(t)$. This implies

$$\begin{aligned} q_\nu(t) + q_\nu(-t) &= \omega_{\nu+1} t \left(\left(t + \frac{1}{2} \right) (t+\nu) - \left(-t + \frac{1}{2} \right) (-t+\nu) \right) \prod_{j=1}^{\nu-1} (t^2 - j^2) \\ &= \omega_{\nu+1} (1+2\nu) t^2 \prod_{j=1}^{\nu-1} (t^2 - j^2), \end{aligned}$$

so that $(-1)^\nu (q_\nu(t) + q_\nu(-t)) \geq 0$, for all $t \in [0, 1]$, from which property **P5** immediately follows. \square

We now have all the instruments for proving the following result.

Proposition 2. For all $\nu \geq 1$, the following inequalities hold true

$$(-1)^{\nu+1} \beta_{2\nu}^{(2\nu)} > 0, \quad (-1)^{\nu+1} (4\beta_{2\nu+2}^{(2\nu+2)} + \beta_{2\nu}^{(2\nu)}) \geq 0. \quad (30)$$

Proof. The first inequality follows immediately from (28) and properties **P1**, **P4** in the previous lemma.

Concerning the second inequality, again from (28) and property **P1**, one gets that it is verified if

$$(-1)^\nu \int_0^1 \int_{-x}^x (p_\nu(t) + p_{\nu+1}(t)) dt dx \geq 0,$$

and this holds true because of property **P5**. \square

We conclude this section with the following result which establishes the type of the second characteristic polynomial $\sigma_{2\nu}(z)$.

Theorem 3. For each $\nu \geq 1$ and $\theta \in [0, 2\pi)$ it results that

$$\sigma_{2\nu}(e^{i\theta}) = (e^{i\theta} + 1)^2 e^{i(\nu-1)\theta} g_{\nu-1}(\theta), \quad (31)$$

where

$$g_{\nu-1}(\theta) = \sum_{j=0}^{\nu-1} (-1)^j \beta_{2j+2}^{(2j+2)} \left(2 \sin \frac{\theta}{2}\right)^{2j} > 0. \quad (32)$$

It follows that $\sigma_{2\nu}(z)$ is of type $(\nu - 1, 2, \nu - 1)$.

Proof. In order to obtain (31)–(32), it is sufficient to consider Remark 1 and to apply Theorem 5.1 in [15] to the sequence of polynomials $(z + 1)^{-2} \sigma_{2\nu}(z)$, $\nu \geq 1$. In addition, from the first inequality in (30), we obtain $g_{\nu-1}(\theta) > 0$. Consequently $\sigma_{2\nu}(z)$ has exactly two roots, namely $z = -1$ with multiplicity 2, of unit modulus. In view of the symmetry of the same polynomial, see (18), we therefore deduce that it is of the indicated type. \square

4. P_ν -stability of PGSCMs

This section is devoted to the proof of the main result of this paper consisting of the P_ν -stability of the family of PGSCMs. As mentioned in Section 2, the main tool we are going to use is the boundary locus (7). We will in fact establish that, for $\theta \in [0, \pi)$, the map $\theta \rightarrow \psi(\theta)$ is one-to-one and onto with respect to the positive semireal axis (origin included). By using this result, we will then prove that the stability polynomial $\pi(z, q^2)$ is of type $(\nu - 1, 2, \nu - 1)$ for all $q^2 \in (0, \infty)$, i.e. that the method is P_ν -stable.

Theorem 4. For each $\nu \geq 1$, let $\rho_{2\nu}(z)$ and $\sigma_{2\nu}(z)$ be the characteristic polynomials of the (2ν) -step PGSCM defined in (9)–(10) with coefficients $\beta_j^{(2\nu)}$'s uniquely determined from (17). Then, the map $\psi : [0, \pi) \rightarrow [0, \infty)$ given by

$$\psi(\theta) = -\frac{\rho_{2\nu}(e^{i\theta})}{\sigma_{2\nu}(e^{i\theta})}$$

is one-to-one and onto.

Proof. From (9) and (31), one immediately gets

$$\begin{aligned} \psi(\theta) &= -\frac{e^{i(\nu-1)\theta} (e^{i\theta} - 1)^2}{(e^{i\theta} + 1)^2 e^{i(\nu-1)\theta} g_{\nu-1}(\theta)} = -\frac{(e^{i\theta/2} - e^{-i\theta/2})^2}{(e^{i\theta/2} + e^{-i\theta/2})^2} \frac{1}{g_{\nu-1}(\theta)} \\ &= \left(\tan \frac{\theta}{2}\right)^2 \frac{1}{g_{\nu-1}(\theta)} \end{aligned}$$

so that the map is onto (recall that, see (32), $g_{v-1}(\theta) > 0$). With the aim of proving that it is also one-to-one, we need to verify that $\psi(\theta)$ is an increasing function for $\theta \in (0, \pi)$. If we let $s(\theta) \equiv \sin^2 \frac{\theta}{2}$ then, see (32),

$$\psi(\theta) = \phi(s(\theta)) \equiv \frac{s(\theta)}{1 - s(\theta)} \frac{1}{g_{v-1}(s(\theta))}, \quad g_{v-1}(s) = \sum_{j=0}^{v-1} (-4)^j \beta_{2j+2}^{(2j+2)} s^j. \quad (33)$$

Clearly, $s(\theta)$ is increasing for $\theta \in (0, \pi)$ so that it is sufficient to prove that

$$\phi'(s) = \frac{g_{v-1}(s) - s(1-s)g'_{v-1}(s)}{((1-s)g_{v-1}(s))^2} > 0$$

or, equivalently, that its numerator is positive. From (33), with some computations, one gets

$$\begin{aligned} (g_{v-1}(s) - sg'_{v-1}(s)) + s^2 g'_{v-1}(s) &= \sum_{j=0}^{v-1} (-4)^j \beta_{2j+2}^{(2j+2)} (1-j)s^j + \sum_{j=2}^v (-1)^j \beta_{2j}^{(2j)} 4^{j-1} (1-j)s^j \\ &= \beta_2^{(2)} + (-4)^{v-1} \beta_{2v}^{(2v)} (v-1)s^v + \sum_{j=2}^{v-1} (-4)^{j-1} (j-1) \left(4\beta_{2j+2}^{(2j+2)} + \beta_{2j}^{(2j)} \right) s^j \end{aligned}$$

which is strictly positive since $\beta_2^{(2)} = 1/4$ and, in view of (30), all the other addends are nonnegative. \square

Theorem 5. For each $v \geq 1$, let $\pi(z, q^2) = \rho_{2v}(z) + q^2 \sigma_{2v}(z)$ be the stability polynomial associated to the $(2v)$ -step PGSCM. Then, for all $q^2 \in (0, \infty)$ the type of $\pi(z, q^2)$ is $(v-1, 2, v-1)$ and the method is P_v -stable when used with $(v+1, v-1)$ -boundary conditions.

Proof. By virtue of the previous theorem and considering that $\pi(z, q^2)$ has real coefficients it is sufficient to observe that, see (7), for all $q^2 \in (0, \infty)$ there exists a unique $\theta \in (0, \pi)$ such that $\pi(e^{i\theta}, q^2) = \pi(e^{-i\theta}, q^2) = 0$. From the symmetry of the method, one therefore gets that the type of $\pi(z, q^2)$ is $(v-1, 2, v-1)$ for all $q^2 > 0$ so that, when used with $(v+1, v-1)$ -boundary conditions, the method is P_v -stable according to Definitions 2 and 3. \square

5. Additional methods and numerical illustrations

The effective use of PGSCMs requires the definition of a suitable strategy for recovering the boundary values in (6). Clearly, the initial value y_0 is provided by the continuous problem. Concerning the remaining ones, we have applied the usual technique for BVMs of getting them implicitly through the application of a set of $2v-2$ additional formulae together with a discretization of the first order derivative $y'(x_0) = y'_0$ at the initial point.

In more detail, if the interval of integration is $[x_0, X]$ and $h = (X - x_0)/N$ then the following set of $v-1$ initial and $v-1$ final additional methods

$$y_{i-1} - 2y_i + y_{i+1} = h^2 \sum_{j=0}^{2v-1} \beta_j^{(i, 2v)} f_j, \quad i = 1, 2, \dots, v-1, \quad (34)$$

$$y_{m-1} - 2y_m + y_{m+1} = h^2 \sum_{j=0}^{2v-1} \beta_j^{(i, 2v)} f_{m-i+j+1}, \quad i = v+1, \dots, 2v-1, \quad m = N + i - 2v \quad (35)$$

are coupled with the main formula in (8). Here, for each $i = 1, 2, \dots, v-1, v+1, \dots, 2v-1$, the coefficients $\beta_j^{(i, 2v)}$'s of the i th additional formula are uniquely determined by imposing it to be of order $2v$, i.e. of the same order as that of the main method.

With reference to the discretization of $y'(x_0)$ we have used a formula analogous to the one considered in [8,23] which is given by

$$-y_0 + y_1 - hy'_0 = h^2 \sum_{j=0}^{2v-1} \beta_j^{(0, 2v)} f_j \quad (36)$$

where again the coefficients are computed in order to keep the same order of the other formulae.

We have applied PGSCMs coupled with (34)–(36) for solving the initial value problem

$$y''(x) = \begin{pmatrix} \mu - 2 & 2\mu - 2 \\ 1 - \mu & 1 - 2\mu \end{pmatrix} y(x), \quad y(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (37)$$

whose exact solution is $y(x) = (2 \cos(x), -\cos(x))^T$ independently of $\mu > 0$. When μ is large, this is a typical example of stiff problem for second order ODEs which is frequently used for testing the performance of P -stable schemes (see, for

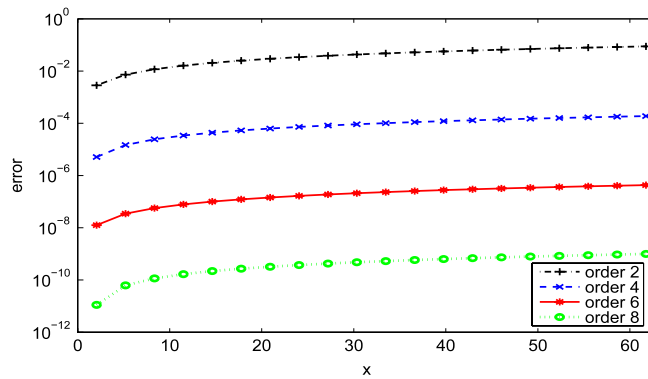


Fig. 1. Error in the approximation of the first component of the solution of Kramar's system.

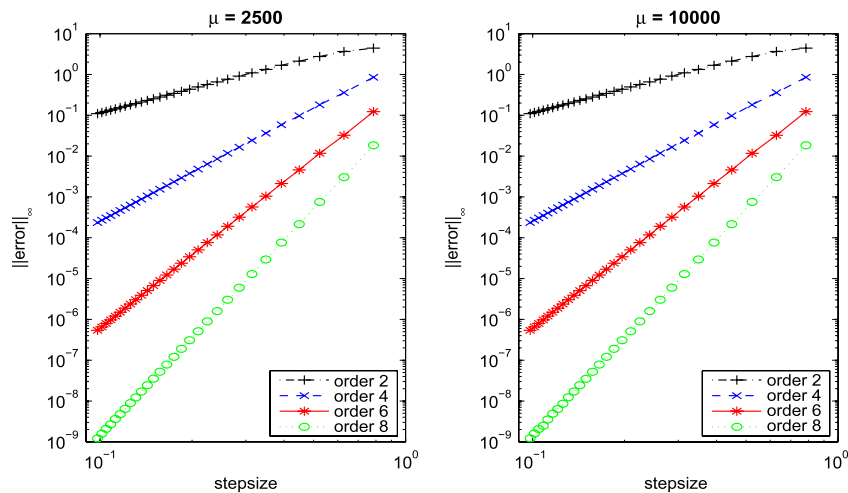


Fig. 2. Error norm (38) versus the stepsize used for problem (37).

example, [10,26]). The eigenvalues of the Jacobian matrix are in fact $-\mu$ and -1 . With the chosen initial value, however, the continuous solution is smooth, i.e. it does not contain modes corresponding to the high frequency. This implies that the system exhibits the phenomenon of *periodic stiffness* so that the application of methods with inappropriate stability properties determines a severe restriction on the choice of the stepsize, [1,2].

We have solved the problem with $\mu = 2500$ (known in the literature as Kramar's system [27]) and $\mu = 10\,000$ over the interval $[0, 20\pi]$ by using the PGSCMs of orders 2, 4, 6, and 8. In Fig. 1, the maximum error over each semi-period for the first component of the solution of Kramar's system obtained with $h = \pi/32$ has been reported. The graphics corresponding to the second component are similar. In Fig. 2, we have plotted

$$\|\text{error}\|_{\infty} = \max_{n=0,1,\dots,N} \|y_n - y(x_n)\|_2, \quad N = \frac{20\pi}{h}, \quad x_n = nh, \quad (38)$$

versus the used stepsize.

As one can see, the figures confirm that the property of P_v -stability of PGSCMs allows to get good approximations of oscillatory solutions of IVPs for second order ODEs even when stiff modes are present and the used stepsize is rather large. Moreover, it is clear that the accuracy of the approximations increases together with the order of the method. Finally, by comparing the two subplots in Fig. 2 one deduces that the error is essentially independent of μ .

Conclusions

In this paper, we have introduced a class of LMMs used as BVMs for solving initial value problems for second order ordinary differential equations having periodic or oscillatory solutions. We have proved theoretically that the new methods are P_v -stable of arbitrarily high order. An interesting topic for future research may be the definition and analysis of a generalized version of PGSCMs in the framework of exponential fitting methods.

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